

2,4,8,10-Tetraoxaspiro[5.5]undecane
126-54-5 | DTXSID2059566

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 5.07 days

Global applicability domain: Outside

Local applicability domain index: 2.19e-01

Confidence level: 8.73e-01

Nearest Neighbors from the Training Set

Image not found

4-Methylheptane

Measured: 24.3

Predicted: 5.24

Image not found

2,2-Dimethylheptane

Measured: 61.9

Predicted: 5.05

Image not found

Pentane, 3-ethyl-

Measured: 24.3

Predicted: 5.29

Image not found

3,3-Dimethylhexane

Measured: 40.7

Predicted: 4.71